Nuclear Instruments and Methods in Physics Research A 649 (2011) 107–108

Contents lists available at ScienceDirect

Nuclear Instruments and Methods in Physics Research A

journal homepage: www.elsevier.com/locate/nima

PID feedback control of monochromator thermal stabilization

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ARTICLE INFO

Available online 9 December 2010

Keywords:
Beamline optics
Thermal stabilization
PID feedback control
Double crystal monochromator

ABSTRACT

The desire for increasingly smaller X-ray beams for macromolecular crystallography experiments also stimulates the need for improvements in beam stability. There are numerous sources of instability, which influence beam quality on the micron-size scale. Typically, the most problematic source is thermal drift within the double crystal monochromators. In addition to using liquid nitrogen to indirectly cool both the first and second crystals, GM/CA-CAT previously used a combination of flowing water at constant temperature and copper braiding to stabilize the mechanics, mounts, and the Compton scatter shielding. However, the copper braids inefficiently stabilized the temperature of components that were distant from the water lines. Additionally, vibrations in the water lines propagated throughout the vibrationally dampened monochromator, thereby introducing both positional and intensity instabilities in the transmitted X-ray beam. To address these problems, heating pads were placed directly onto the temperature-sensitive components, with output controlled by a PID-feedback loop. As a result, there is negligible temperature change in the first crystal radiation shielding over the entire range of operational heat loads. Additionally, the angular drift in the second crystal induced by temperature changes in other components is dramatically decreased.

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Recently, there has been considerable interest in the use of micron and sub-micron X-ray beams for macromolecular crystallography, both to tailor the beam to the sample size and to reduce radiation damage during the experiment [1–5]. At the General Medicine and Cancer Institutes Collaborative Access Team (GM/CA-CAT, Sector 23, Advanced Photon Source) users are routinely provided with beam sizes as small as 5 μm, and sub-micron beams have been used for radiation damage research [6–8]. Producing these small beams with low convergence required by the large unit cell dimensions (up to 100 nm) of biological macromolecules places increased demands on the stability of the various beamline components. In particular, instabilities that cause angular fluctuations are particularly troublesome, since small deviations in the desired angle may cause large motions given the typical distance between the optics and the sample. Within monochromators, there is the potential for angular fluctuations, as well as an extreme environment caused by high undulator power loading. Extra care must be taken to stabilize those environments.

The GM/CA-CAT beamlines were constructed by ACCEL Instruments (now Bruker AXS Corporation) with design input on managing the high heat load based on the previous experience of GM/CA personnel. As a result of this collaborative effort and the ongoing developments, the monochromators on the two insertion device beamlines have very high thermal stability. They are capable of accepting the full closed-gap power of the APS Undulator A (approximately 600 W through the premask), while undergoing a temperature increase of only 40 °C (vs. dark conditions) in the Compton scatter shield around the first crystal (the maximum increase in all other components is significantly less). Additionally, the optics were designed to handle the additional heat load arising from increasing the storage ring current from 100 to 200 mA [9].

The performance of the monochromators is excellent, with only a 1% rms intensity fluctuation observed through a 10-μm beam-defining slit (oriented to be sensitive to vertical motion) at the sample location. However, the flow of water through the lines within the monochromator introduced vibrations into the system, thereby increasing the noise in the delivered X-ray beam to 2% (see Fig. 1). In addition to this noise increase, heat flow from the water lines through the copper braiding was inefficient, leading to some long equilibration times.

Although the circulating water was initially intended to cool the mechanics under high-heat-load conditions, it was found to be keeping several components of the monochromators from cooling below room temperature through direct conduction or indirect Blackbody radiation. The liquid nitrogen that was cooling the crystals was also cooling the entire system (albeit inefficiently). Even under closed-gap undulator conditions, the cooling from the liquid nitrogen had a greater effect than the heat load from the insertion device. Therefore, we concluded that the circulating water could be removed and replaced by installing resistive heating pads directly onto sensitive monochromator components. By choosing a temperature setpoint slightly above the maximum temperature attained under high heat load, PID feedback control could be used to control the output heating power. When exposed to a high

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doi:10.1016/j.nima.2010.11.177

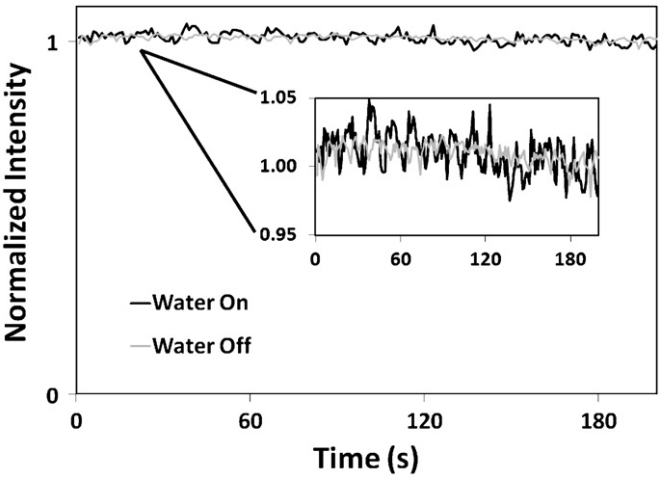

Fig. 1. Noise in the intensity of the focused beam through a 10-μm slit at the sample position. Inset expands the vertical scale to more clearly show the increase in noise when the water is flowing.

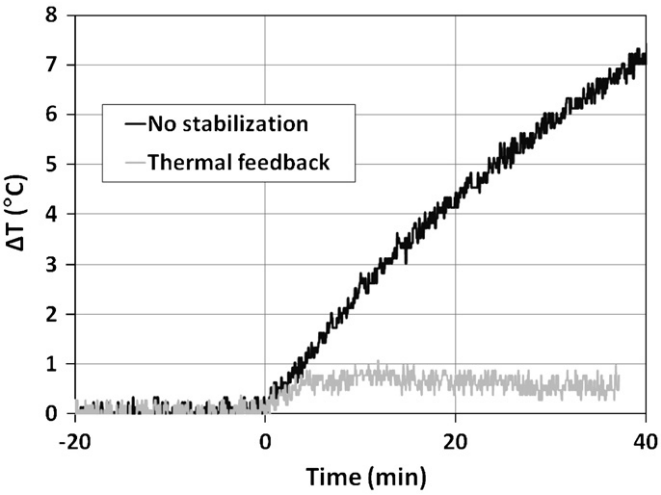

Fig. 2. Temperature increase in the Compton shielding around the first monochromator crystal when undergoing an energy change from 12 to 6 keV.

power output from the undulator, the temperature feedback is able to reduce the power to the heaters, thereby maintaining a constant temperature at the point of control.

Flexible polyimide-coated heaters as well as the needed controllers were purchased from the Watlow Electric Manufacturing Company. Initially, three locations were identified for temperature control: the Compton scatter shielding around the first crystal, the mounting bracket of the first crystal, and the mounting bracket of the second crystal. The Compton shielding was chosen because of the large amount of heat that is re-radiated from its surface. The two mount positions were chosen because thermal drift in those locations induces angular changes (roll of the first crystal or pitch of the second) that have the potential to move the beam.

Initial results are promising. Although the impact of these changes on the stability of the focused beam at the sample position has not been measured, the thermal response of the targeted components is improved. For example, there is a substantial decrease observed in time that the Compton scatter shielding requires for equilibration. When the 23-ID-B monochromator energy is changed from 12 to 6 keV, the power on the first Si-111 crystal is increased by about 150 W. Without thermal feedback, the equilibrium temperature on the first crystal Compton shielding increased by 13 °C with a time constant of approximately 48 min. However, with the feedback implemented, the temperature change was less than 1 °C with a time constant below 2 min (see Fig. 2).

To simulate the effect of shielding temperature changes on other parts of the monochromator in the absence of an X-ray load, a 13 °C increase was applied to the Compton scatter shielding, while the pitch angle of the second crystal was monitored via encoder. Without temperature feedback, the pitch angle changed by 36 μrad—an amount slightly larger than the Si-111 rocking curve width (FWHM) at 12 keV. With feedback, however, the change was reduced by two-thirds to 11 μrad. However, in both cases, the time constant of the change was quite long (11.5 h) presumably due to poor thermal conductivity between the location of the heater and the second crystal mount (see Fig. 3).

The ability to decrease both the equilibration time and the temperature change of key components of the monochromator during a change in power load is encouraging, as is the decreased influence of the temperature of one part of the monochromator on another. The influence of these modifications on the stability of the delivered X-ray beam will be tested soon, and investigations to improve the current performance are ongoing. Ultimately, the goal is to develop beamline stability of $<0.5\%$ rms for routine use with sub-micron beams for macromolecular crystallography.

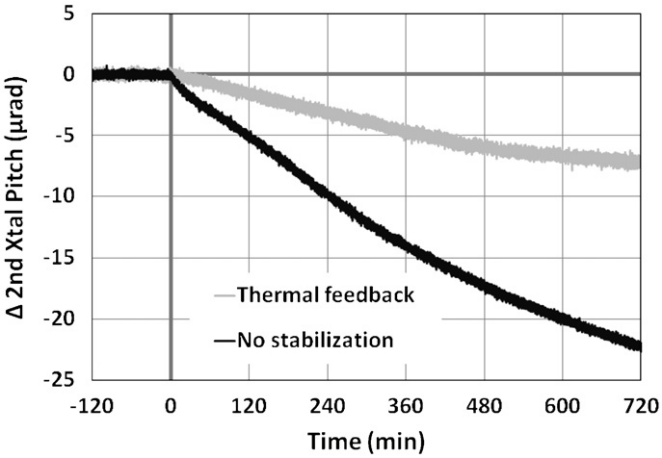

Fig. 3. Drift in the second monochromator crystal pitch angle associated with a 13 °C increase in the temperature of the Compton shielding around the first crystal. Drift is measured by the pitch encoder.

GM/CA CAT is funded with Federal funds from the National Cancer Institute (Y1-CO-1020) and the National Institute of General Medical Science (Y1-GM-1104). Use of the Advanced Photon Source was supported by the U.S. Department of Energy, Basic Energy Sciences, Office of Science, under contract no. DE-AC02-06CH11357.

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